Proposal: CRG-2741		2741	<b>Council:</b> 10/2019				
Title:	Adsor	Adsorption to biomimetic hair surface					
Research	area: Soft co	ondensed matter					
This propos	al is a new p	roposal					
Main proposer:		Mark RUTLAND					
Experimental team:		Alexei VOROBIEV					
		Mark RUTLAND					
Local contacts:		Alexei VOROBIEV					
Samples:	D2O						
	NaCl						
	Deuterated s	sodium dodecyl sulphate					
	-	icosanoic acid					
	polyethylim	ine					
Instrument			Requested days	Allocated days	From	То	
SUPERADAM			5	5	08/02/2021	09/02/2021	
					15/06/2021	19/06/2021	

The project is designed to study adsorption to the lipid palisade that forms the boundary of hair. Strategies for robust, hierarchical adsorption are limited by lack of understanding of how the lipid density and the amount of methyl branching affect the attachment, and by the difficulty of direct study of hair. Such knowledge is crucial for the design of protective and restorative coatings. Neutron reflectance provides the ideal experimental window to understand how the unique branching of hair lipids affects self-assembly and adsorption in water. It is ideal for understanding hierarchical adsorption, where deuteration will provide the contrast. This is particularly crucial in the current climate where there is an urgent need for new, sustainable materials to replace conventional additives which had years of optimisation. The studies will be supported by AFM and in-situ adsorption studies in Sweden. Adsorption models for coadsorbing polymers and surfactant to lipid surfaces based on Self-Consistent Field Theory exist, but these models require experimental verification and refinement.

## Experimental report for proposal CRG-2741

From 15/06/21 to 19/06/21 on SuperADAM

The performed experiments aimed at characterizing the adsorption of surfactants and polymers to biomimetic hair surfaces produced by self-assembly of thiols on gold. This information is important for the cosmetic industry to improve the formulation of hair care products.

These experiments are part of the thesis work for the InnovaXN PhD project of Serena Cozzolino "Adhesion and interaction with hair biomolecules – a cosmetic perspective".

A lipid layer covers the hair surface and makes it hydrophobic. Its major component is the molecule 18-methyl eicosanoic acid (18-MEA); damaged hair has a reduced lipid coverage and is hydrophilic.

Two types of surfaces have been produced by using commercial thiols with relevant features:

1. Octadecanethiol (ODT) layer – long, straight chain giving a hydrophobic surface; two experiments were planned on this kind of surface

2. 2-methyl-1-butanethiol layer - short, branched thiol, which reproduces the characteristic antepenultimate methyl branch found in 18-MEA

Both surfaces are hydrophobic, but the methyl branch affects chain packing. The experiments here were designed to understand how this difference in packing influences adsorption.

One of the ODT surfaces, and the surface with the short, branched thiol, have been characterized in:

- gold contrast matched water (GMW, 74:26 D<sub>2</sub>O:H<sub>2</sub>O) plus 100 mM NaCl (similar ionic strength of real formulations), before and after the injection of the solutions below
- deuterated sodium dodecyl sulfate (dSDS) at the concentrations of 0.1, 0.5 and 2 cmc in GMW
- 20 cmc or 2 cmc dSDS + 100 ppm polymer in GMW (the polymer was pDADMAC for the ODT surface and chitosan for the other surface)

For the second ODT surface, the explored conditions were:

- GMW, before and after the injection of the solutions below
- hydrogenous SDS at the concentrations of 0.1, 0.5 and 2 cmc
- 2 cmc dSDS in GMW or GMW plus 100 mM NaCl, pH 4.5
- 20 cmc dSDS + 100 ppm chitosan in GMW + 100 mM NaCl, pH 4.5
- Final rinse with pure  $D_2O$  to check from the critical edge in the NR curve that solvent replacement is complete

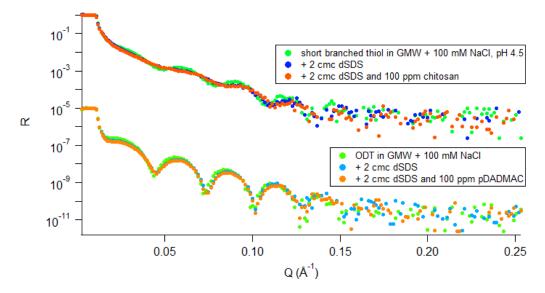


Figure 1. NR curves of the thiol surfaces, in GMW and after adsorption of dSDS or dSDS/polymer mixture. The change in the signal is different depending on the examined surface.

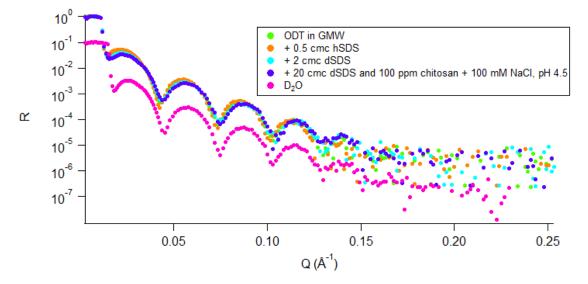


Figure 2. NR curves of the ODT surfaces produced for the third experiment, in GMW and after adsorption of hydrogenous (h-) or deuterated (d-) SDS or dSDS/chitosan mixture. Deuteration allows to better distinguish SDS adsorption. The shift of the critical edge after the final rinse with  $D_2O$  proves that the injection of a new solution effectively replaces the previous one present in the cell.